# SAT Report for Case # P-17-0023

## General

**CBI:** [redacted]

**Report Status:** Complete **Status Date:** 11/03/2016

**CRSS Date:** 11/03/2016 **SAT Date:** 11/04/2016 **SAT Chair:** [redacted]

**Consolidated PMN?**

**Consolidated Set:**

**Submitter:** [redacted]

**CAS Number:** 1072-53-3

**Ecotox Related Cases:** [redacted]

**Health Related Cases:** [redacted]

**Chemical Name:** 1,3,2-Dioxathiolane, 2,2-dioxide

**Use:** Additive for use in lithium ion battery electrolyte formulations. [redacted]

**Trade name:** ESA, DTD

**PV Max (kg/yr):**

**Ecotox Assessor:** [redacted] **Fate Assessor:** [redacted] **Health Assessor:** [redacted]

## Physical Chemical Information

| | | | | | |
|---|---|---|---|---|---|
| **Molecular Weight:** | 124.12 | **Physical State - Neat:** | Solid | | |
| **Percent 500:** | | **Percent 1000:** | | | |
| **Melting Point (Measured):** | 95.00 - 97.00 | **Melting Point (est):** | | **MPD (EPI):** | |
| **Vapor Pressure:** | | **Vapor Pressure (est):** | 0.043 | **VP (EPI):** | |
| **Water Solubility:** | | **Water Solubility (EST):** | 407 | **Water Solubility (EPI):** | |
| **Log Kow:** | | | | **Log Kow (EPI):** | |
| **Log P:** | | **Log P Comment:** | | | |

## SAT Concern

| | | | |
|---|---|---|---|
| **Ecotox Rating (1):** | 2 | **Ecotox Rating Comment (1):** | |
| **Ecotox Rating (2):** | | **Ecotox Rating Comment (2):** | |
| **Health Rating (1):** | 2 | **Health Rating Comment (1):** | |
| **Health Rating (2):** | | **Health Rating Comment (2):** | |

## PBT Ratings

| Persistence | Bioaccumulation | Toxicity | Comments |
|---|---|---|---|
| 3 | 1 | 2 | |

| | |
|---|---|
| **Exposure Based Review (Health)?** | |
| **Exposure Based Review (Ecotox)?** | N |
| **SAT Keywords:** | SEVER IRR/CORR.E, S, L, SENS.S, ACUTE, LIVER, DEVEL, MUTA, ONCO |

**Fate Assessment Summary:** P-17-0023

FATE:
Solid with MP = 95-97 °C (M)

log Kow = -0.90 (E)
S > 10 g/L at 25 °C (E)
VP = 4.4E-2
torr at 25 °C (E)
BP = 209 °C (E)
H = 1.15E-6 (E)
log Koc =
0.97 (E)
log Fish BCF = 0.50 (3) (E)
log Fish BAF = -0.05 (1) (E)

POTW removal (%) = 0-25 via possible biodeg
Time for complete
ultimate aerobic biodeg = wk
Sorption to soils/sediments = low

Volatilization half-life from a standard river = 570 hrs

Volatilization half-life from a standard lake = 260 da
Atmospheric
Oxidation Half-life = 120 hr via OH radical
PBT Potential: P3B1

*CEB FATE: Migration to ground water = rapid

Overall
wastewater treatment removal is 0-25% based analogous chemicals.

Sorption to sludge is low based on analogous chemicals.
Air
Stripping (Volatilization to air) is low based on analogous chemicals and the estimated vapor pressure.
Removal by biodegradation in wastewater

| | |
|---|---|
| | treatment is negligible to moderate based on analogous chemicals and BIOWIN model estimates.<br>The aerobic aquatic biodegradation half-life is weeks based on analogous chemicals.<br>The anaerobic aquatic biodegradation half-life is months to greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.<br>Sorption to soil and sediment is low based on PCKOC model estimates and analogous chemicals.<br>Migration to groundwater is rapid based on the estimated water solubility and analogous chemicals.<br>PMN Material:<br>High Persistence (P3) is based on the anaerobic biodegradation half-life.<br>Low Bioaccumulation potential (B1) is based on analogous chemicals. |
| **Removal in WWT/POTW (Overall):** | 0-25 |

| Condition | Rating Values<br><br>w/ Rating Description | Comment |
|---|---|---|
| **WWT/POTW Sorption:** | 1 | |
| **WWT/POTW Stripping:** | 3 | |
| **Biodegradation Removal:** | 3-4 | |
| **Biodegradation Destruction:** | | |
| **Aerobic Biodeg Ult:** | 2 | |
| **Aerobic Biodeg Prim:** | | |
| **Anaerobic Biodeg Ult:** | 3-4 | |
| **Anaerobic Biodeg Prim:** | | |
| **Hydrolysis (t1/2 at pH 7,25C) A:** | | |

| Condition | Rating Values w/ Rating Description | Comment |
|---|---|---|
| **Hydrolysis (t1/2 at pH 7,25C) B:** | | |
| **Sorption to Soils/Sediments:** | 4 | |
| **Migration to Ground Water:** | 4 | |
| **Photolysis A, Direct:** | | |
| **Photolysis B, Indirect:** | | |
| **Atmospheric Ox A, OH:** | | |
| **Atmospheric Ox B, O3:** | | |

## Health Assessment

**Health Summary:** Absorption is nil through the skin for the neat material, moderate through the skin for the material in solution, and moderate through the lung and GI tract, based on physical/chemical properties. The PMN is a potential alkylating agent. There are concerns for severe irritation/possible corrosion to the eye, skin, and lung, dermal sensitization, acute, liver and developmental toxicities, mutagenicity, and oncogenicity, based on the alkylation potential.

**Routes of Exposure:** Dermal Drinking Water Inhalation

## Test Data Submitted

**Test Data Submitted:** Test data on the PMN substance: Test Data: Submitted with [redacted]

## Ecotox Assessment

| Test organism | Test Type | Test Endpoint | Predicted | Measured | Comments |
|---|---|---|---|---|---|
| **Fish** | 96-h | LC50 | >100 | >15.2 | |
| **Daphnid** | 48-h | LC50 | >100 | >12.4 | |
| **Green Algae** | 96-h | EC50 | >100 | >9.1 | |
| **Fish** | - | Chronic Value | >10 | | |
| **Daphnid** | - | Chronic Value | >10 | | |
| **Green Algae** | - | Chronic Value | >10 | 5 | |

| Factors | Most Sensitive Endpoint | Assessment Factor | CoC | Comment |
|---|---|---|---|---|
| **Acute Acquatic:** | | 4 | 5000 | acute/chronic |
| **Chronic Acquatic:** | | 10 | 500 | acute/chronic |

| | |
|---|---|
| **Ecotox Route of Exposure?** | All releases to water |

| Factors | Values | Comments |
|---|---|---|
| **SARs:** | esters | |
| **SAR Class:** | esters | |
| **TSCA NCC Category?** | Esters | |

## Recommended Testing

## Ecotox

## Value Comments

Predictions are based on SARs for esters; SAR chemical class = ester; MW 124; solid with mp = 97 C (M); S = 38.2 g/L at 20 C (P); pH7; effective concentrations based on 100% active ingredients and nominal concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;

Acute base set toxicity testing was submitted [redacted] that was considered an acceptable study method, but did not test to a high enough concentration.

Focus Report/Decision Document:
Environmental Hazard
and Risk
(P-17-0023)

Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model) and hazard data for the new chemical substance. Based on these estimated hazard values from ECOSAR and hazard values from test data for the new chemical substance, EPA concludes that this chemical substance has moderate environmental hazard.

· Substance falls within the TSCA New Chemicals Category of Esters.

· ECOSAR chemical class of esters.
· High hazard based on acute and chronic concentrations of concern of 5,000 ppb and 500 ppb, respectively.

F ish Ecotoxicity Test:

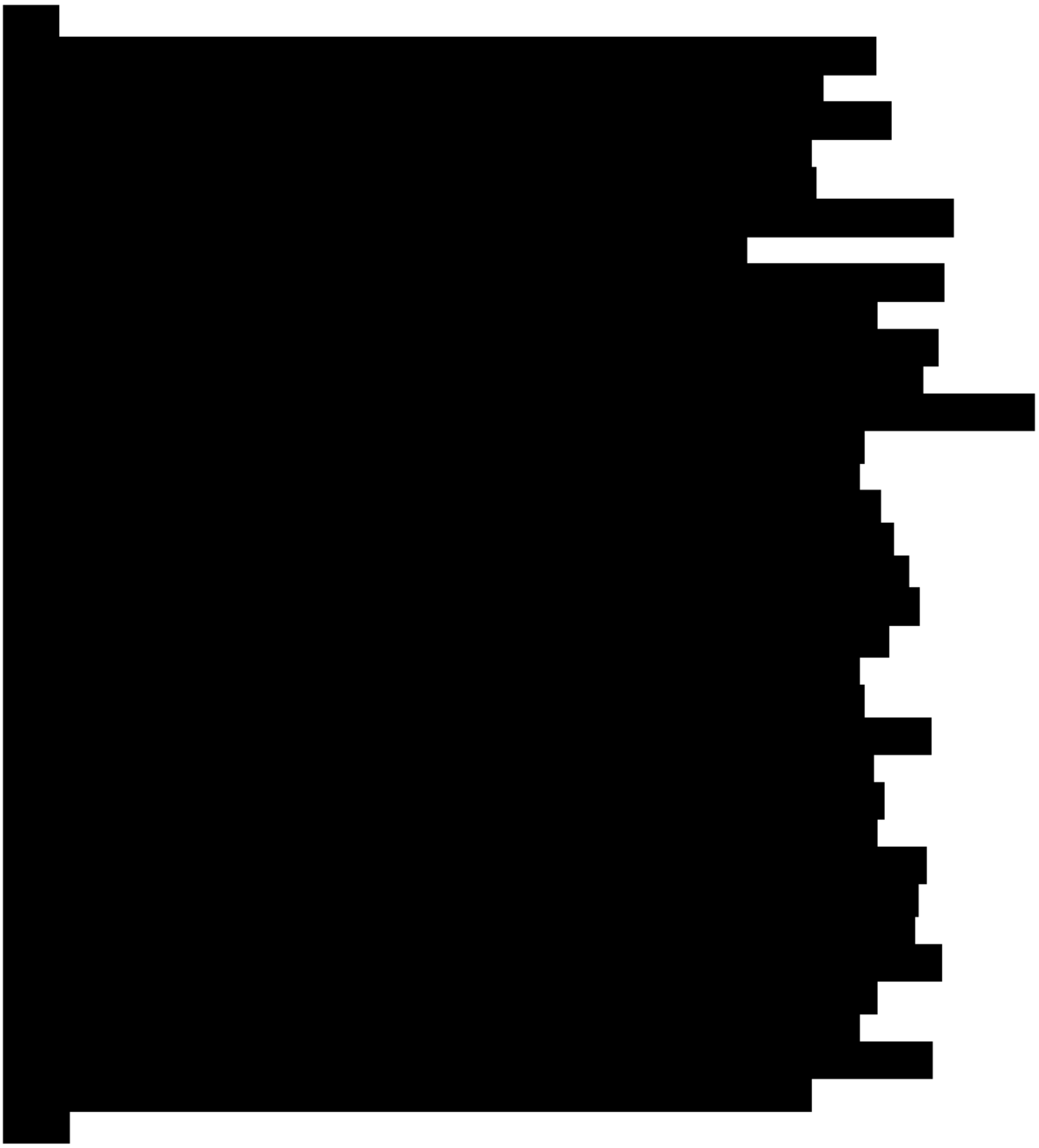
[redacted]

Daphnid Ecotoxicity Test:

[redacted]

48-hour EC50 > 12.429 mg/L

Algal Ecotoxicity



72-hour EC50 (yield) > 9.068 mg/L
72-hour LOEC
(yield) = 3.41 mg/L
72-hour EC50 (growth rate) > 9.068 mg/L
72-hour
NOEC (growth rate) = 4.43 mg/L
72-hour LOEC (growth rate) = 5.59 mg/L

72-hour ChV (growth rate) = 4.98 mg/L

[redacted]

Ecotox Study Reviewer: [redacted]

**Ecotox**
**Factors Comments**